

SCHRÖDINGER OPERATORS ON EXTERIOR DOMAINS WITH ROBIN BOUNDARY CONDITIONS: HEAT KERNEL ESTIMATES

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ABSTRACT. We study Schrödinger operators with Robin boundary conditions on exterior domains in \mathbb{R}^d . We prove sharp point-wise estimates for the associated semigroups which show, in particular, how the boundary conditions affect the time decay of the heat kernel in dimensions one and two. Applications to spectral estimates are discussed as well.

1. Introduction

In this paper we consider Laplace operators with Robin boundary conditions defined on domains of the type $M = \mathbb{R}^d \setminus K$, where $K \subset \mathbb{R}^d$ is an open bounded set. Given a bounded function $\sigma : \partial M \rightarrow \mathbb{R}$ we consider the Laplace operator $-\Delta_\sigma$ in $L^2(M)$ defined by means of the sesquilinear form

$$Q_\sigma[u, v] = \int_M \nabla \bar{u} \cdot \nabla v \, dx + \int_{\partial M} \sigma \bar{u} v \, dS, \quad u, v \in H^1(M). \quad (1.1)$$

Note that the above form with $\sigma = 0$ generates the Neumann Laplacian $-\Delta_0$ on $L^2(M)$. The standard theory of Gaussian heat kernel estimates, see e.g. [Gr, Thms. 6.1, 6.2] or [SC, Sect. 4.2], implies that there exist positive constants c and $C > 0$ such that the semigroup generated by $-\Delta_0$ satisfies

$$C^{-1} t^{-\frac{d}{2}} e^{-\frac{c|x-y|^2}{t}} \leq e^{t\Delta_0}(x, y) \leq C t^{-\frac{d}{2}} e^{-\frac{|x-y|^2}{ct}} \quad \forall x, y \in M, \quad t > 0. \quad (1.2)$$

The goal of this paper is to show that if $\sigma > 0$ and $d \leq 2$, then the heat kernel generated by the Robin Laplacian $-\Delta_\sigma$ decays faster than the heat kernel of the Neumann Laplacian $-\Delta_0$ and to establish sharp estimates on the decay rate.

In order to quantify the effect of the boundary term in (1.1) we will work in a more general setting and consider Schrödinger operators in $L^2(M)$ of the type

$$H_\sigma(\lambda, U) = -\Delta_\sigma - \lambda U,$$

(to be interpreted in a weak sense as a form sum), where $U : M \rightarrow \mathbb{R}$ is a real-valued positive function and $\lambda > 0$ is a coupling constant. Under suitable conditions on U , see Corollary 2.5 below, the operator $-H_\sigma(\lambda, U)$ generates a semigroup on $L^2(M)$ given by an integral kernel which we denote by

$$e^{-tH_\sigma(\lambda, U)}(x, y), \quad x, y \in M.$$

We will pay particular attention to the case $d = 2$ which is studied in detail in section 2. Our aim is to prove that the presence of Robin boundary conditions accelerates the decay of $e^{-tH_\sigma(\lambda, U)}(x, y)$ in such a way that if $U > 0$ belongs to a certain potential class and if λ

Key words and phrases. Heat kernel, Robin boundary conditions, exterior domains, Schrödinger operators.
Version of April 11, 2016.

is small enough, then the semigroup $e^{-tH_\sigma(\lambda, U)}$ results transient. This is in sharp contrast to the case of Neumann boundary conditions. i.e. $\sigma = 0$, where the associated semigroup $e^{-tH_0(\lambda, U)}$ is recurrent even for $\lambda = 0$ as follows from equation (1.2) with $d = 2$.

The decay of the heat kernel generated by $H_\sigma(\lambda, U)$ depends, apart from the boundary conditions, also on the potential U . Hence in order to establish sharp heat kernel bounds we will assume that U can be controlled by the reference potential

$$U_\sigma(x) := \frac{1}{4|x|^2} \left(\log \frac{|x|}{\rho} + \frac{1}{\rho\sigma_0} \right)^{-2}, \quad (1.3)$$

where ρ is the in-radius of K and σ_0 is the essential infimum of σ . More precisely, we will show that if $U \leq U_\sigma$ and if $\lambda \leq 1$, then the heat kernel satisfies

$$e^{-tH_\sigma(\lambda, U)}(x, y) = \mathcal{O} \left(t^{-1} (\log t)^{-1-\sqrt{1-\lambda}} \right) \quad t \rightarrow \infty, \quad (1.4)$$

point-wise for all $x, y \in M$, see Theorem 2.6 for details. The logarithmic factor, which makes the heat kernel decay faster with respect to (1.2), reflects the effect of the boundary conditions. On the other hand, the presence of the negative potential $-\lambda U$ is reflected by the term $\sqrt{1-\lambda}$ in the power of the logarithm.

Similarly, if $U \geq U_\sigma$ then the heat kernel is bounded below by a function which has the same decay in t as the right hand side of equation (1.4), see Proposition 2.13. In other words, the decay rate in t in estimate (1.4) is sharp. A two-sided estimate on the heat kernel in the case $U = U_\sigma$ is established in Theorem 2.16. The latter implies, in particular, that the semigroup $e^{-tH_\sigma(\lambda, U_\sigma)}$ is transient for $\lambda < 1$ and recurrent for $\lambda = 1$.

Operators with Dirichlet boundary conditions at ∂M are discussed in section 2.4, see Theorem 2.10. We use the fact that Dirichlet boundary conditions can be achieved as a limiting case of the Robin ones by changing the form domain in (1.1) to $H_0^1(M)$ and subsequently letting $\sigma \rightarrow +\infty$. The reference potential (1.3) then takes the form

$$U_\infty(x) := \frac{1}{4|x|^2} \left(\log \frac{|x|}{\rho} \right)^{-2}. \quad (1.5)$$

For heat kernel estimates of Dirichlet Laplacians, without an additional negative potential, in unbounded domains, and in particular in exterior domains, we refer to [GS, Zh02, Zh03].

The proof of our main results relies upon transforming the problem to an analysis of a Neumann Laplacian in suitable weighted L^2 -spaces with a λ -dependent weight. We then employ the technique of the Li-Yau type heat kernel estimates on weighted manifolds invented by Grigor'yan and Saloff-Coste, see [Gr, GS] or [SC, Chap. 4] and references therein. In section 3 we discuss some applications of the obtained heat kernel bounds to Hardy and Hardy-Lieb-Thirring inequalities for Schrödinger operators on exterior two-dimensional domains.

Although we are primarily interested in semigroups generated by Robin Laplacians in dimension two, we discuss the analogous problem in other dimensions as well. It turns out that while the effect of the boundary on the decay rate of the associated heat kernel is even stronger in dimension one, see Theorem 4.1, in dimensions larger than two it is absent. Although the latter assertion is well-known for Dirichlet heat kernels, [GS], for the sake of self-containdness we state an analogous result for Robin Laplacians in Proposition 5.1.

2. The case $d = 2$

Throughout Sections 2 and 3 we will work under the following conditions on the potential U , the exterior domain M and the coefficient σ in the Robin boundary conditions.

Assumption 2.1. There exists $p \in [2, \infty)$ such that $U \in L^p(\mathbb{R}^2) + L^\infty(\mathbb{R}^2)$. In other words $U = U_1 + U_2$ with $U_1 \in L^p(\mathbb{R}^2)$, $p \geq 2$, and $U_2 \in L^\infty(\mathbb{R}^2)$.

Assumption 2.2. The set $K \subset \mathbb{R}^2$ is open, bounded and simply connected with Lipschitz boundary; we let $M := \mathbb{R}^2 \setminus K$.

Assumption 2.3. The coefficient σ lies in $L^\infty(\partial M)$ and we denote by

$$\sigma_0 := \text{ess inf}_{\partial M} \sigma$$

its essential infimum on ∂M .

2.1. Preliminaries.

Lemma 2.4. Assume σ to be non-negative. Then the sesquilinear form

$$\tilde{Q}_{\sigma, \lambda}[u, v] = \int_M \nabla \bar{u} \cdot \nabla v \, dx - \lambda \int_M U \bar{u} v \, dx + \int_{\partial M} \sigma \bar{u} v \, dS \quad (2.1)$$

defined on $H^1(M) \times H^1(M)$ is closed in $L^2(M)$ for all $\lambda \in \mathbb{R}$.

Proof. Let $u, v \in H^1(M)$ and moreover let $p \geq 2$ be as in assumption 2.1. Under the regularity assumptions on K it follows from standard Sobolev imbedding theorems and trace inequalities, see e.g. [AdaFou, Thm. 4.12 and Thm. 5.36] that there exists a constant $C_q > 0$ such that

$$\|f\|_{L^q(\partial M)} \leq C_q \|f\|_{H^1(M)}, \quad \|f\|_{L^q(M)} \leq C_q \|f\|_{H^1(M)} \quad (2.2)$$

hold true for all $f \in H^1(M)$, all $q \in [2, \infty)$. Hence by the assumption on U and Hölder inequality we have

$$\begin{aligned} \left| \int_{\partial M} \sigma u v \, dS \right| &\leq \|\sigma\|_\infty C_M^2 \|u\|_{H^1(M)} \|v\|_{H^1(M)} \\ \left| \int_M U u v \, dx \right| &\leq C_q \|U_1\|_p \|u\|_{H^1(M)} \|v\|_{H^1(M)} + C_2 \|U_2\|_\infty \|u\|_{H^1(M)} \|v\|_{H^1(M)}. \end{aligned}$$

This shows that

$$|\tilde{Q}_{\sigma, \lambda}[u, v]| \leq C \|u\|_{H^1(M)} \|v\|_{H^1(M)}. \quad (2.3)$$

In order to prove a suitable lower bound on $\tilde{Q}_{\sigma, \lambda}[v, v]$ we recall the Gagliardo-Nirenberg inequality

$$\|f\|_q \leq K_q \|f\|_2^{\frac{2}{q}} (\|\nabla f\|_2 + \|f\|_2)^{1 - \frac{2}{q}} \quad \forall f \in H^1(M) \quad (2.4)$$

which holds for all $q \in [2, \infty)$, see e.g. [AdaFou, Thm. 5.8]. This and the Young inequality:

$$AB \leq \frac{\delta^r}{r} A^r + \frac{\delta^{-r'}}{r'} B^{r'}, \quad A, B > 0, \quad \frac{1}{r} + \frac{1}{r'} = 1, \quad \delta > 0, \quad (2.5)$$

implies that for every $\varepsilon > 0$ there exists a constant $c_1(\varepsilon)$ such that

$$\|f\|_q^2 \leq \varepsilon \|\nabla f\|_2^2 + c_1(\varepsilon) \|f\|_2^2 \quad \forall f \in H^1(M). \quad (2.6)$$

Thus, similarly as above, we can use the Hölder inequality to get

$$\begin{aligned} \left| \int_M U v^2 dx \right| &\leq \|U_1\|_p \|v\|_q^2 + \|U_2\|_\infty \|v\|_2^2 \\ &\leq \varepsilon \|U_1\|_p \|\nabla v\|_2^2 + (\|U_1\|_p c_1(\varepsilon) + \|U_2\|_\infty) \|v\|_2^2 \end{aligned}$$

Now if we choose ε small enough, then we conclude that the lower bound

$$\tilde{Q}_{\sigma,\lambda}[v, v] + \|v\|_2^2 \geq c \|v\|_{H^1(M)},$$

holds for some $c > 0$ and all $v \in H^1(M)$. In view of (2.3) this completes the proof. \square

In the sequel we denote by $H_\sigma(\lambda, U)$ the unique self-adjoint and positive operator on $L^2(M)$ associated with the sesquilinear form $\tilde{Q}_{\sigma,\lambda}[\cdot, \cdot]$. As a consequence of the above lemma we obtain

Corollary 2.5. *If σ is non-negative, then the operator $H_\sigma(\lambda, U)$ generates on $L^2(M)$ a sub-Markovian semigroup given by an integral kernel.*

Proof. The form $\tilde{Q}_{\sigma,\lambda}$ is symmetric and, by Lemma 2.4, also closed. Moreover, a direct computation shows that the Beurling-Deny conditions are satisfied, hence the operator $-H_\sigma(\lambda, U)$ generates on $L^2(M)$ an analytic sub-Markovian semigroup. By the Sobolev embedding theorem, cf. [Bre, Cor. 9.14], $H^1(M) \hookrightarrow L^q(M)$ for all $q \in [2, \infty)$. Thus, the semigroup is ultracontractive and is hence given by an integral kernel of class $L^\infty(M \times M)$, see e.g. [Are, § 7.3.2–7.3.3]. \square

2.2. Notation. In the sequel we denote by $B(x, r) \subset \mathbb{R}^d$ a ball of radius r centered in x . Let $\rho > 0$ be the in-radius of K :

$$\rho = R_{\text{in}}(K) := \sup_{y \in K} \text{dist}(y, \partial K). \quad (2.7)$$

Without loss of generality we may choose the coordinate system in such a way that

$$B(0, \rho) \subseteq K. \quad (2.8)$$

We denote by $-\Delta_D$ the Dirichlet Laplacian in $L^2(M)$.

2.3. Heat kernel upper bounds. Throughout this section, our techniques rely upon the assumption that the parameter σ_0 introduced in Assumption 2.3 satisfies

$$\sigma_0 > 0.$$

We have

Theorem 2.6. *In addition to the Assumption 2.2, let $K \subset \mathbb{R}^2$ have C^2 -regular boundary. Let $\rho > 0$ be given by (2.7) and let $\sigma_0 > 0$. Suppose moreover that*

$$U(x) \leq \frac{1}{4|x|^2} \left(\log \frac{|x|}{\rho} + \frac{1}{\rho \sigma_0} \right)^{-2} \quad \forall x \in M, \quad (2.9)$$

and that $\lambda \in [0, 1]$. Then there exist positive constants c, C such that for all $x, y \in M$ and all $t > 0$

$$e^{-tH_\sigma(\lambda, U)}(x, y) \leq \frac{C \left(\log \frac{|x|}{\rho} + \frac{1}{\rho\sigma_0} \right)^{\frac{1+\sqrt{1-\lambda}}{2}} \left(\log \frac{|y|}{\rho} + \frac{1}{\rho\sigma_0} \right)^{\frac{1+\sqrt{1-\lambda}}{2}} e^{-\frac{|x-y|^2}{ct}}}{t \left(\log \left(\frac{|x|+\sqrt{t}}{\rho} \right) + \frac{1}{\rho\sigma_0} \right)^{1+\sqrt{1-\lambda}}}. \quad (2.10)$$

Remark 2.7. The condition $\lambda \leq 1$ is necessary. Indeed, if K is a ball, then the operator $H_\sigma(\lambda, U_\sigma)$ is not positive for $\lambda > 1$, see Proposition 3.1.

Proof of Theorem 2.6. Our assumptions on K imply that there exists a mapping $N : [0, 2\pi] \rightarrow \mathbb{N}$ and C^2 -regular functions $R_j, S_j : [0, 2\pi] \rightarrow [0, \infty]$ such that

$$R_j(\theta) \leq S_{j+1}(\theta) \leq R_{j+1}(\theta) \quad \forall j = 0, 1, \dots, N(\theta), \quad \forall \theta \in [0, 2\pi], \quad (2.11)$$

and

$$K = \left\{ (r \cos \theta, r \sin \theta) : \theta \in [0, 2\pi], r \in [0, R_0(\theta)) \cup \bigcup_{j=1}^{N(\theta)} (S_j(\theta), R_j(\theta)) \right\}. \quad (2.12)$$

In particular, K is star-shaped if and only if $N(\theta) = 0$ for all $\theta \in [0, 2\pi]$. Moreover, by assumption the curvature of ∂K is bounded. Hence

$$\sup_{\theta \in [0, 2\pi]} N(\theta) < \infty. \quad (2.13)$$

Next we define the weight function

$$w(x) := \left(\log \frac{|x|}{\rho} + \beta \right)^\alpha, \quad x \in M, \quad (2.14)$$

where $\alpha \in \mathbb{R}$ and $\beta \in \mathbb{R}$ are two positive parameters whose values will be specified later. Since w is positive on M , we can write any test function $u \in H^1(M)$ as a product

$$u(x) = w(x) f(x), \quad (2.15)$$

for some

$$f \in H^1(M, w^2 dx) := \left\{ f \in H^1(M) : \int_M (|\nabla f|^2 + |f|^2) w^2 dx < \infty \right\}. \quad (2.16)$$

Let $A_\sigma(\lambda, U)$ be the self-adjoint operator in $L^2(M, w^2 dx)$ associated with the closed quadratic form

$$Q_\sigma[wf, wf] - \lambda \int_M U |f|^2 w^2 dx, \quad f \in H^1(M, w^2 dx), \quad (2.17)$$

which by the Beurling-Deny criteria generates a sub-Markovian semigroup on $L^2(M, w^2 dx)$. As already mentioned, in order to show that this semigroup has a kernel it suffices to prove its ultracontractivity; by [Are, Thm. in § 7.3.2] this is in turn equivalent to showing that the imbedding $H^1(M, w^2 dx) \hookrightarrow L^{\frac{2m}{m-2}}(M, w^2 dx)$ is continuous for some $m > 2$ – this is done in Lemma B.1. Let now $e^{-tA_\sigma(\lambda, U)}(x, y)$ be the integral kernel of this semigroup. Note that the mapping $f \mapsto wf$ is an isometry from $L^2(M, w^2 dx)$ onto $L^2(M, dx)$. Hence in view of (2.15) it follows that

$$e^{-tH_\sigma(\lambda, U)}(x, y) = w(x) w(y) e^{-tA_\sigma(\lambda, U)}(x, y), \quad \forall x, y \in M, \quad t > 0. \quad (2.18)$$

We can write the sesquilinear form $Q_\sigma[u, v]$ in polar coordinates as

$$\begin{aligned} Q_\sigma[u, v] &= \int_0^{2\pi} \sum_{j=1}^{N(\theta)} \int_{S_j(\theta)}^{R_j(\theta)} (\partial_r \bar{u} \partial_r v + r^{-2} \partial_\theta \bar{u} \partial_\theta v) r dr d\theta \\ &\quad + \int_0^{2\pi} \sum_{j=1}^{N(\theta)} \sigma(R_j(\theta), \theta) (\bar{u} v)(R_j(\theta), \theta) \sqrt{R_j^2(\theta) + (R_j'(\theta))^2} d\theta \\ &\quad + \int_0^{2\pi} \sum_{j=1}^{N(\theta)} \sigma(S_j(\theta), \theta) (\bar{u} v)(S_j(\theta), \theta) \sqrt{S_j^2(\theta) + (S_j'(\theta))^2} d\theta. \end{aligned} \quad (2.19)$$

Let us factorize u, v as $u = wf$ and $v = wg$, with $f, g \in H^1(M, w^2 dx)$. Now assume that $f, g \in H^1(M, w^2 dx)$ are real and positive; we are going to show that

$$Q_\sigma[wf, wg] - \lambda \int_M U f g w^2 dx \geq \int_M \nabla f \cdot \nabla g w^2 dx =: \widehat{Q}_\sigma[f, g]. \quad (2.20)$$

Since w is radial, cf. (2.14), we have $\partial_\theta(wf) = w \partial_\theta f$ and $\partial_\theta(wg) = w \partial_\theta g$. On the other hand, for the radial derivatives we obtain

$$\begin{aligned} \partial_r u \partial_r v &= \left(\log \frac{r}{\rho} + \beta \right)^{2\alpha} \partial_r f \partial_r g + \frac{\alpha^2}{r^2} \left(\log \frac{r}{\rho} + \beta \right)^{2\alpha-2} f g \\ &\quad + \frac{\alpha}{r} (f \partial_r g + g \partial_r f) \left(\log \frac{r}{\rho} + \beta \right)^{2\alpha-1}. \end{aligned}$$

Next we use the shorthands $R_j(\theta) = R_j$, $S_j(\theta) = S_j$ and integrate the last term by parts with respect to r . This gives

$$\begin{aligned} \int_{S_j}^{R_j} \partial_r u \partial_r v r dr &= \int_{S_j}^{R_j} \left(\log \frac{r}{\rho} + \beta \right)^{2\alpha} \partial_r f \partial_r g r dr + \alpha \left(\log \frac{R_j}{\rho} + \beta \right)^{2\alpha-1} (fg)(R_j, \theta) \\ &\quad - \alpha \left(\log \frac{S_j}{\rho} + \beta \right)^{2\alpha-1} (fg)(S_j, \theta) \\ &\quad + (\alpha - \alpha^2) \int_{S_j}^{R_j} r^{-1} \left(\log \frac{r}{\rho} + \beta \right)^{2\alpha-2} f g dr. \end{aligned} \quad (2.21)$$

We emphasize that this formula is valid for all $\alpha, \beta \in (0, \infty)$. Let us now fix the parameters α, β : we take

$$\alpha = \frac{1 + \sqrt{1 - \lambda}}{2}, \quad \beta = \frac{1 + \sqrt{1 - \lambda}}{2\rho\sigma_0}, \quad (2.22)$$

and plug (2.21) into (2.19). Keeping in mind the upper bound (2.9) and the fact that by (2.8)

$$R_j(\theta) \geq \rho \quad \forall j = 0, \dots, N(\theta), \quad \forall \theta \in [0, 2\pi],$$

we conclude that the inequality (2.20) holds for all positive functions $f, g \in H^1(M, w^2 dx)$.

Denote by \widehat{A}_σ the self-adjoint operator in $L^2(M, w^2 dx)$ associated with the sesquilinear form \widehat{Q}_σ with form domain $H^1(M, w^2 dx)$. The operator \widehat{A}_σ acts on its domain, in the sense of distributions, as

$$\widehat{A}_\sigma u = w^{-2} \nabla \cdot (w^2 \nabla u). \quad (2.23)$$

It is easy to see that if a real-valued function f lies in $H^1(M, w^2 dx)$, then so do its positive part f^+ and the function $f \wedge 1$ and in particular both Beurling-Deny conditions are satisfied

and accordingly the generated semigroups $e^{-tA_\sigma(\lambda, U)}$ and $e^{-t\hat{A}_\sigma}$ are sub-Markovian, [Ouh, Cor. 2.18]. Moreover the form domains of $A_\sigma(\lambda, U)$ and \hat{A}_σ coincide. Hence in view of (2.20) we can apply [Ouh, Thm. 2.24] which implies that the semigroup generated by $-A_\sigma(\lambda, U)$ is dominated by the semigroup generated by $-\hat{A}_\sigma$ and hence

$$e^{-tA_\sigma(\lambda, U)}(x, y) \leq e^{-t\hat{A}_\sigma}(x, y) \quad \forall x, y \in M, \quad \forall t > 0. \quad (2.24)$$

Now consider the weighted manifold $(M, w^2 dx)$ endowed with the Euclidean metric. For any $x \in M$ we denote by $B(x, \sqrt{t})$ the ball of radius \sqrt{t} centered in x . Let

$$\mathcal{V}_2(x, \sqrt{t}) := \int_{B(x, \sqrt{t}) \cap M} w^2(y) dy \quad (2.25)$$

be the volume, in $(M, w^2 dx)$, of the intersection of $B(x, \sqrt{t})$ with M . Given any $x_0 \in M$ it is easily verified that the pointed manifold (M, x_0) satisfies the condition of relatively connected annuli, see e.g. [GS, Def. 2.10]. Moreover, in view of (2.14) there exists a constant C_h , independent of λ and σ , such that

$$\sup_{x \in B(x_0, 2r)} w(x) \leq C_h \inf_{x \in M \setminus B(x_0, r)} w(x) \quad (2.26)$$

holds for all r large enough, see Lemma A.1. We may thus apply [GS, Thm. 2.11] with $d\mu = dx$ and $d\nu = w^2 dx$, which implies that $(M, w^2 dx)$ satisfies the parabolic Harnack inequality. In view of [GS, Thm. 2.8] this further yields the following two-sided estimate on the heat kernel of \hat{A}_σ ;

$$\frac{C_1 e^{-\frac{c|x-y|^2}{t}}}{\mathcal{V}_2(x, \sqrt{t})} \leq e^{-t\hat{A}_\sigma}(x, y) \leq \frac{C_2 e^{-\frac{|x-y|^2}{ct}}}{\mathcal{V}_2(x, \sqrt{t})}, \quad x, y \in M, \quad C_1, C_2, c > 0. \quad (2.27)$$

Since

$$\mathcal{V}_2(x, \sqrt{t}) \geq c_0 t \left(\log \left(\frac{|x| + \sqrt{t}}{\rho} \right) + \beta \right)^{2\alpha} \quad (2.28)$$

by Lemma A.2, see Appendix A, equations (2.22) and (2.27) in combination with (2.18) and (2.24) imply the claim. \square

Remark 2.8. Since the weighted manifold $(M, w^2 dx)$ satisfies the volume doubling property, cf. Lemma A.3, the denominator on the right hand side of (2.10) may be replaced by either

$$t \left(\log \left(\frac{|x| + \sqrt{t}}{\rho} \right) + \frac{1}{\rho\sigma_0} \right)^{\frac{1+\sqrt{1-\lambda}}{2}} \left(\log \left(\frac{|y| + \sqrt{t}}{\rho} \right) + \frac{1}{\rho\sigma_0} \right)^{\frac{1+\sqrt{1-\lambda}}{2}},$$

or

$$t \left(\log \left(\frac{|y| + \sqrt{t}}{\rho} \right) + \frac{1}{\rho\sigma_0} \right)^{1+\sqrt{1-\lambda}}$$

This follows from [GS, Lem. 2.4, Rem. 2.7] and Lemma A.2.

Remark 2.9. Semigroups generated by Schrödinger operators

$$-\Delta + Q \quad \text{in } L^2(\mathbb{R}^d)$$

were studied by several authors. Potentials which satisfy $Q(x) = -c|x|^{-2}$ outside a compact set were considered by Grigor'yan in [Gr, Sec. 10.4] for $d \geq 2$. The case $Q = -c|x|^{-2}$ with

$c \leq \frac{(d-2)^2}{4}$ and $d \geq 3$ was treated later in [MS1, MS2]. In both cases it was proved that the decay rate of the heat kernel depends on c .

On the other hand, compactly supported positive potentials Q were considered by Murata for $d = 2$, see [M84]. He showed in particular that if Q is Hölder continuous then

$$e^{-t(-\Delta+Q)}(x, y) \asymp \frac{\varphi(x)\varphi(y)}{t(\log t)^2}, \quad t \rightarrow \infty, \quad (2.29)$$

where the function φ satisfies $\varphi(x) = \log|x|(1+o(1))$ as $x \rightarrow \infty$. This is compatible with (2.10) for $\lambda = 0$. It is also interesting to notice that the same point-wise decay as in (2.29) was observed for magnetic Laplace operators in \mathbb{R}^2 associated with radial magnetic fields of zero integral mean, see [Ko].

Finally we point out that heat kernel upper bounds for elliptic operators with (nonlocal) Robin-type boundary conditions on bounded domains were recently obtained in [GMN, GMNO].

2.4. Dirichlet boundary conditions. A straightforward modification of Lemma 2.4 shows that the sesquilinear form

$$Q_\infty[u, v] - \lambda \int_\Omega U \bar{u} v \, dx = \int_M \nabla \bar{u} \cdot \nabla v \, dx - \lambda \int_\Omega U \bar{u} v \, dx, \quad u, v \in H_0^1(M) \quad (2.30)$$

is closed in $L^2(M)$ whenever U satisfies assumption 2.1. Let $H_D(\lambda, U)$ be the self-adjoint operator in $L^2(M)$ associated with the form (2.30). Hence $H_D(\lambda, U)$ is subject to Dirichlet boundary conditions at ∂M . Our next result provides an upper bound on the semigroup generated by $H_D(\lambda, U)$.

Theorem 2.10. *Let $\lambda \in [0, 1]$. Then there exist positive constants C, c such that for all $t > 0$ and all $x, y \in M$ we have*

$$e^{-tH_D(\lambda, U_\infty)}(x, y) \leq \frac{C \left(\log \frac{|x|}{\rho} \right)^{\frac{1+\sqrt{1-\lambda}}{2}} \left(\log \frac{|y|}{\rho} \right)^{\frac{1+\sqrt{1-\lambda}}{2}} e^{-\frac{|x-y|^2}{ct}}}{t \left(\log \frac{|x|+\sqrt{t}}{\rho} \right)^{1+\sqrt{1-\lambda}}} \quad (2.31)$$

Remark 2.11. Note that the potential U_∞ defined in (1.5) belongs to $L^p(M)$ for any $p \in [1, \infty)$ and therefore satisfies assumption 2.1.

The heat kernel estimate in (2.31) is the precise counterpart of the estimate (2.10) *as the Robin boundary conditions of $-\Delta - \lambda U$ tend to the Dirichlet ones*, i.e. as $\sigma_0 \rightarrow +\infty$. This is not yet a precise argument, but our proof will actually refine this observation.

Proof of Theorem 2.10. We consider the sequence of quadratic forms

$$q_n[u, u] = \int_M |\nabla u|^2 \, dx - \lambda \int_M U_{\frac{1}{n}} |u|^2 \, dx, \quad u \in H_0^1(M), \quad (2.32)$$

and the corresponding self-adjoint operators $h_n(\lambda)$ in $L^2(M)$ associated with q_n . Then

$$h_n(\lambda) \geq h_{n+1}(\lambda) \geq H_D(\lambda, U_\infty) \geq 0, \quad \forall n \in \mathbb{N},$$

where the last inequality follows from Corollary 3.3 below. Since

$$\lim_{n \rightarrow \infty} q_n[u, u] = Q_\infty[u, u] - \lambda \int_\Omega U_\infty |u|^2 \, dx \quad \forall u \in H_0^1(M),$$

by the monotone convergence theorem, we conclude that $h_n(\lambda)$ converges to $H_D(\lambda, U_\infty)$ in the strong resolvent sense, see e.g. [Da2, Thm. 1.2.3]. Hence for each $t > 0$ the semigroup $e^{-th_n(\lambda)}$ converges strongly to $e^{-tH_D(\lambda, U_\infty)}$ as $n \rightarrow \infty$. On the other hand, the domination of semigroups and Theorem 2.6 imply that

$$e^{-th_n(\lambda)}(x, y) \leq e^{-tH_{\frac{n}{\rho}}(\lambda, U_{1/n})}(x, y) \leq \frac{C \left(\log \frac{|x|}{\rho} + \frac{1}{n} \right)^{\frac{1+\sqrt{1-\lambda}}{2}} \left(\log \frac{|y|}{\rho} + \frac{1}{n} \right)^{\frac{1+\sqrt{1-\lambda}}{2}} e^{-\frac{|x-y|^2}{ct}}}{t \left(\log \left(\frac{|x|+\sqrt{t}}{\rho} \right) + \frac{1}{n} \right)^{1+\sqrt{1-\lambda}}}$$

holds for all $t > 0$ and all $x, y \in M$. Hence follows by passing to the limit $n \rightarrow \infty$ we conclude that (2.31) holds almost everywhere in M . The continuity of $e^{-tH_D(\lambda, U_\infty)}(x, y)$ with respect to x, y then implies (2.31) for all $x, y \in M$. \square

Remark 2.12. Consider the case of the two-dimensional unit ball $K = B(0, 1)$. If we put $\lambda = 0$, then $H_D(0, U_\infty)$ coincides with the pure Dirichlet Laplacian $-\Delta_D$ and our upper bound (2.31) gives

$$e^{t\Delta_D}(x, x) \leq \frac{c \log^2 |x|}{t (\log(|x| + \sqrt{t}))^2}, \quad c > 0,$$

which agrees with the two-sided estimate

$$\frac{\log^2 |x|}{C t (\log(1 + \sqrt{t}) + \log |x|)^2} \leq e^{t\Delta_D}(x, x) \leq \frac{C \log^2 |x|}{t (\log(1 + \sqrt{t}) + \log |x|)^2} \quad (2.33)$$

obtained in [GS, Eq. (1.8)] for $|x|$ large enough. To see this we note that

$$\frac{1}{2} \left(\log(1 + \sqrt{t}) + \log |x| \right) \leq \log(|x| + \sqrt{t}) \leq \log(1 + \sqrt{t}) + \log |x|$$

holds for all $x \in M$ and $t > 0$. Indeed, since $|x| > 1$, we have

$$\begin{aligned} 2 \log(|x| + \sqrt{t}) &= \log(|x|^2 + 2|x|\sqrt{t} + t) \geq \log(|x| + |x|\sqrt{t}), \\ &= \log(1 + \sqrt{t}) + \log |x|, \end{aligned}$$

and on the other hand

$$\log(1 + \sqrt{t}) + \log |x| = \log(|x| + |x|\sqrt{t}) \geq \log(|x| + \sqrt{t}).$$

Hence the factor $\log(1 + \sqrt{t}) + \log |x|$ in (2.33) can be replaced by $\log(|x| + \sqrt{t})$.

2.5. Heat kernel lower bounds. In order to establish a lower bound on the heat kernel of $H_\sigma(\lambda, U)$ we obviously need a lower bound on the potential U . We will thus assume that

$$U(x) \geq \frac{1}{4|x|^2} \left(\log \frac{|x|}{\rho} + \beta \right)^{-2}, \quad (2.34)$$

holds for some $\beta > 0$ and all $x \in M$. Moreover, for a given $\delta > 0$ we introduce the external δ -neighborhood

$$K_\delta := \{x \in M : \text{dist}(x, K) < \delta\} \quad (2.35)$$

of K .

Proposition 2.13. *Let K have a C^2 -boundary and assume that U satisfies (2.34) for some $\beta > 0$. Let $0 \leq \lambda < 1$. Then there exist $\varepsilon > 0$ and $c, C > 0$ such that*

$$e^{-tH_\sigma(\lambda, U)}(x, y) \geq \frac{C \left(\log \frac{|x|}{\rho} + \beta \right)^{\frac{1+\sqrt{1-\lambda}}{2}} \left(\log \frac{|y|}{\rho} + \beta \right)^{\frac{1+\sqrt{1-\lambda}}{2}} e^{-\frac{c|x-y|^2}{t}}}{t \left(\log \left(\frac{|x|+\sqrt{t}}{\rho} \right) + \beta \right)^{1+\sqrt{1-\lambda}}} \quad (2.36)$$

holds for all $x, y \in M \setminus K_\varepsilon$ and all $t > 0$.

Proof. Let $\Omega = M \setminus \partial K$. By domination of semigroups

$$e^{-tH_\sigma(\lambda, U)}(x, y) \geq e^{-tH_D(\lambda, U)}(x, y) \quad \forall x, y \in \Omega, \quad t > 0. \quad (2.37)$$

Now we mimic the proof of Theorem 2.6 and write $u = wf$, $v = wg$ with w as in (2.14) and

$$f, g \in H_0^1(\Omega, w^2 dx) = \{f \in H_0^1(\Omega) : w(|\nabla f| + |f|) \in L^2(\Omega)\}.$$

Let \widehat{Q}_∞ be the sesquilinear form on $H_0^1(\Omega, w^2 dx) \times H_0^1(\Omega, w^2 dx)$ defined by

$$\widehat{Q}_\infty[f, g] = \int_\Omega \nabla \bar{f} \cdot \nabla g \, w^2 dx.$$

Now the boundary terms in (2.21) vanish and for all positive functions $f, g \in H_0^1(\Omega, w^2 dx)$ we obtain the lower bound

$$\begin{aligned} Q_\infty[wf, wg] - \lambda \int_\Omega U fg w^2 dx &\leq Q_\infty[wf, wg] - \lambda \int_\Omega \frac{1}{4|x|^2} \left(\log \frac{|x|}{\rho} + \beta \right)^{-2} fg w^2 dx \\ &= \widehat{Q}_\infty[f, g]. \end{aligned} \quad (2.38)$$

By [Ouh, Thm. 2.24] and (2.18) this gives

$$e^{-tH_D(\lambda, U)}(x, y) \geq w(x)w(y) e^{-t\widehat{A}_\infty}(x, y) \quad \forall x, y \in M, \quad (2.39)$$

where \widehat{A}_∞ is the operator in $L^2(\Omega, w^2 dx)$ associated with the form $\widehat{Q}_\infty[\cdot, \cdot]$ with the form domain $H_0^1(M, w^2 dx)$. Note that since $\lambda < 1$, it follows from Lemma A.2 that

$$\int_0^\infty \frac{dt}{\mathcal{V}_2(x, \sqrt{t})} < \infty \quad \forall x \in M.$$

Hence the manifold $(M, w^2 dx)$ is non-parabolic. Since ∂K is compact and $(M, w^2 dx)$ satisfies the parabolic Harnack inequality, see the proof of Theorem 2.6, we may apply [GS, Thm. 3.1] with $(M, \mu) = (M, w^2 dx)$ and Ω as above. The latter says that there exists $\varepsilon > 0$ such that

$$e^{-t\widehat{A}_\infty}(x, y) \geq C' e^{-c' t \widehat{A}_\sigma}(x, y), \quad t > 0, \quad x, y \in M \setminus K_\varepsilon,$$

holds for some $c', C' > 0$. Here \widehat{A}_σ is the operator in $L^2(M, w^2 dx)$ defined in (2.23). From (2.27) and Lemma A.2 we thus obtain

$$e^{-t\widehat{A}_\infty}(x, y) \geq \frac{C' C_1 e^{-\frac{c|x-y|^2}{t}}}{\mathcal{V}_2(x, \sqrt{t})} \geq \frac{C' C_1 e^{-\frac{c|x-y|^2}{t}}}{\pi t \left(\log \left(\frac{|x|+\sqrt{t}}{\rho} \right) + \beta \right)^{1+\sqrt{1-\lambda}}}. \quad (2.40)$$

To complete the proof it suffices to apply (2.39) to the right hand side of (2.40). \square

Remark 2.14. For $\lambda = 1$ the weighted manifold $(M, w^2 dx)$ becomes parabolic, see (2.14) and (2.22). Hence the Dirichlet heat kernel $e^{-t\hat{A}_\infty}(x, y)$ in this case has a faster decay in t than the upper bound (2.10). Indeed, by [GS, Thm. 4.9]

$$e^{-t\hat{A}_\infty}(x, x) \asymp \frac{1}{t \log t \log(\log t)} \quad t \rightarrow \infty$$

holds for all x far enough from K . This forbids an extension of Proposition 2.13 to the case $\lambda = 1$.

Remark 2.15. A slightly more general notion of Gaussian estimates for a semigroup with kernel $k(t, x, y)$ consists in the inequality

$$|k(t, x, y)| \leq C t^{-\frac{d}{2}} e^{-\frac{|x-y|^2}{bt}} e^{\omega t}$$

for some constants $b, c > 0$ and $\omega \in \mathbb{R}$ and all $t > 0$ as well as almost every x, y . The advantage of this formulation is that also semigroups with complex-valued kernels can be discussed. Now, it is well-known that the semigroup generated by a (formal) Schrödinger operator $\Delta - V$ with potential $V \in L^p_{\text{loc}}$ such that $\text{Re} V \geq 0$ admits a modulus semigroup (i.e., a minimal dominating semigroup), which is then generated by $\Delta - \text{Re} V$. This suggests a slight generalisation of Proposition 2.13: the estimate (2.36) accordingly holds if the kernel $e^{-tH_\sigma(\lambda, U)}(x, y)$ on the left hand side is replaced by its complex absolute value, provided U is a complex-valued potential that satisfies $\text{Re} U(x) \geq U_\beta(x)$ for some $\beta > 0$ and all $x \in M$.

2.6. A two-sided estimate. Here we provide a two-sided heat kernel estimate for $U = U_\sigma$.

Theorem 2.16. *Let $K \subset \mathbb{R}^2$ be an open bounded and simply connected set with C^2 regular boundary. Let $0 \leq \lambda < 1$. Then there exist positive constants $C, c > 0$ and $\varepsilon > 0$ such that for all $x, y \in M \setminus K_\varepsilon$ and all $t > 0$ we have*

$$\frac{F_2(x, y; \lambda) e^{-\frac{c|x-y|^2}{t}}}{Ct \left(\log \left(\frac{|x|+\sqrt{t}}{\rho} \right) + \frac{1}{\rho\sigma_0} \right)^{1+\sqrt{1-\lambda}}} \leq e^{-tH_\sigma(\lambda, U_\sigma)}(x, y) \leq \frac{C F_2(x, y; \lambda) e^{-\frac{|x-y|^2}{ct}}}{t \left(\log \left(\frac{|x|+\sqrt{t}}{\rho} \right) + \frac{1}{\rho\sigma_0} \right)^{1+\sqrt{1-\lambda}}}, \quad (2.41)$$

where

$$F_2(x, y; \lambda) := \left(\left(\log \frac{|x|}{\rho} + \frac{1}{\rho\sigma_0} \right) \left(\log \frac{|y|}{\rho} + \frac{1}{\rho\sigma_0} \right) \right)^{\frac{1+\sqrt{1-\lambda}}{2}}.$$

Proof. The claim follows from Theorem 2.6 and Proposition 2.13. \square

Note that both upper and lower bound in (2.41) are decreasing functions of σ_0 .

Remark 2.17. For small times the diagonal element of the behavior of the heat kernel is not affected by the presence of the boundary, neither by the potential U_σ . In fact

$$e^{-tH_\sigma(\lambda, U_\sigma)}(x, x) \asymp t^{-1} \quad t \rightarrow 0.$$

On the other hand, for large times we have

$$e^{-tH_\sigma(\lambda, U_\sigma)}(x, x) \asymp t^{-1} (\log t)^{-1-\sqrt{1-\lambda}} \quad t \rightarrow \infty.$$

Remark 2.18. Consider the case $\sigma = \text{const}$ and $\lambda = 0$. To simplify the notation we write H_σ instead of $H_\sigma(0, U_\sigma)$. By domination of semigroups we then have

$$e^{-tH_D}(x, x) \leq e^{-tH_\Sigma}(x, x) \leq e^{-tH_\sigma}(x, x) \leq e^{-tH_0}(x, x) \quad x \in M \setminus K_\varepsilon, \quad (2.42)$$

for all $0 < \sigma < \Sigma$. By passing to the limit $\sigma \rightarrow 0$ in (2.41), for a fixed $x \in M \setminus K_\varepsilon$, we thus obtain

$$e^{-tH_0}(x, x) \asymp t^{-1} \quad (\text{Neumann boundary conditions}) \quad (2.43)$$

Remark 2.19. There are two reasons why Theorem 2.16 is not completely satisfactory. First, the lower bound is non-zero only for x far enough from K . This is because we use the Dirichlet heat kernel as a bound from below, see (2.37) and (2.39). Second, it does not cover the critical case $\lambda = 1$, see Remark 2.14 for details. Both these artifacts can be removed in the special case when $K = B(0, \rho)$ and σ is constant. This suggests that the assertion of Theorem 2.16 might actually be improved.

Example: a ball with constant σ .

Proposition 2.20. *Let $K = B(0, \rho)$, $\sigma = \sigma_0$ and let U be as in Theorem 2.16. Then the two-sided estimate (2.41) holds for all $x, y \in M$ and all $\lambda \in [0, 1]$.*

Proof. Take w as in (2.14) with α and β given by (2.22). We then obtain the identity

$$Q_\sigma[wf, wg] - \lambda \int_M U \bar{f} g w^2 dx = \hat{Q}_\sigma[f, g], \quad (2.44)$$

where $\hat{Q}_\sigma[\cdot, \cdot]$ is defined in (2.20). The above equation holds for all functions $f, g \in H^1(M, w^2 dx)$. Hence

$$e^{-tH_\sigma(\lambda, U)}(x, y) = w(x)w(y)e^{-t\hat{A}_\sigma}(x, y), \quad \forall x, y \in M, \quad t > 0.$$

The claim now follows from (2.27) and Lemma A.2. \square

3. Applications

In this section we will apply the heat kernel bounds obtained in section 2.3 to establish spectral estimates for two-dimensional Schrödinger operators on exterior domains. We begin with a simple but important consequence of the proof of Theorem 2.6.

3.1. A Hardy inequality.

Proposition 3.1. *In addition to the Assumption 2.1, let $K \subset \mathbb{R}^2$ have C^2 -regular boundary. Then for all $u \in H^1(M)$ it holds*

$$Q_\sigma[u, u] \geq \frac{1}{4} \int_M \frac{|u(x)|^2}{|x|^2 \left(\log \frac{|x|}{\rho} + \frac{1}{2\rho\sigma_0} \right)^2} dx, \quad (3.1)$$

where $Q_\sigma[\cdot, \cdot]$ is given by (1.1). Moreover, the above inequality fails if we replace the constant $\frac{1}{4}$ on the right hand side by any constant $C > \frac{1}{4}$.

Proof. As above we write

$$u(x) = \left(\log \frac{|x|}{\rho} + \frac{1}{2\rho\sigma_0} \right)^{\frac{1}{2}} f(x). \quad (3.2)$$

Inequality (3.1) then follows immediately from (2.20) applied with $\lambda = 1$. To prove the sharpness of the constant $1/4$ we consider the example $K = B(0, 1)$ and $\sigma = \sigma_0 > 0$ treated already in Proposition 2.20. Using the factorization (3.2) with a radial test function u we then obtain the following identity;

$$\begin{aligned} Q_\sigma[u, u] - C \int_M \frac{|u(x)|^2}{|x|^2 \left(\log \frac{|x|}{\rho} + \frac{1}{2\rho\sigma_0} \right)^2} dx &= 2\pi \int_1^\infty (f'(r))^2 r \left(\log r + \frac{1}{2\rho\sigma_0} \right) dr \\ &\quad - 2\pi \left(C - \frac{1}{4} \right) \int_1^\infty f^2(r) r^{-1} \left(\log r + \frac{1}{2\rho\sigma_0} \right)^{-1} dr. \end{aligned} \quad (3.3)$$

If we now set

$$f(r) = f_n(r) = \begin{cases} \log \left(\log \left(1 - \log \frac{r}{n} \right) + 1 \right) & \text{if } r \leq n, \\ 0 & \text{if } n < r \end{cases} \quad n \in \mathbb{N},$$

then $f_n \in H^1(M)$ and a direct calculation shows that the right hand side of (3.3) is negative for n large enough whenever $C > 1/4$. \square

Remark 3.2. Hardy-type inequalities for Laplace operators with Robin boundary conditions were recently established in [KL]. Among other things it was shown in [KL, Thm. 5.1] that for a constant σ the inequality

$$Q_\sigma[u, u] \geq \frac{1}{4} \int_M \left(\left(|x| - \rho + \frac{1}{2\sigma} \right)^{-2} + \frac{(d-1)(d-3)}{|x|^2} \right) |u(x)|^2 dx \quad (3.4)$$

holds for all $u \in H^1(M)$, where $M = \mathbb{R}^d \setminus B(0, \rho)$. Note however, for $d = 2$ the integral weight on the right hand side of (3.4) is positive only for σ large enough. Moreover, still for $d = 2$, this weight decays as $|x|^{-3}$ for $|x| \rightarrow \infty$, whereas the integral weight in (3.1) has the optimal decay rate $|x|^{-2} (\log |x|)^{-2}$.

Corollary 3.3. *In addition to the Assumption 2.1, let $K \subset \mathbb{R}^2$ have C^2 -regular boundary. Then for all $u \in H_0^1(M)$ it holds*

$$\int_M |\nabla u|^2 dx \geq \frac{1}{4} \int_M \frac{|u(x)|^2}{|x|^2} \left(\log \frac{|x|}{\rho} \right)^{-2} dx, \quad (3.5)$$

with the sharp constant $1/4$.

Proof. In view of the monotone convergence theorem the claim follows by applying (3.1) to $u \in H_0^1(M)$ and letting $\sigma_0 \rightarrow \infty$. \square

3.2. Hardy-Lieb-Thirring inequalities. It is well known that the Laplace operator satisfies, in the sense of quadratic forms on $H^1(\mathbb{R}^d)$, the Hardy inequality

$$-\Delta \geq \frac{(d-2)^2}{4|x|^2} \quad d \geq 3, \quad (3.6)$$

with the sharp constant $(d-2)^2/4$. Motivated by this fact Ekholm and Frank established in [EF] the so-called Hardy-Lieb-Thirring inequalities, i.e. estimates for the moments of negative eigenvalues $\{-\lambda_j(V)\}$ of a Schrödinger operator $-\Delta - \frac{(d-2)^2}{4|x|^2} - V$ in terms of a suitable L^p -norm of V . More precisely, they proved that

$$\mathrm{Tr} \left(-\Delta - \frac{(d-2)^2}{4|x|^2} - V \right)_-^\gamma = \sum_j \lambda_j(V)^\gamma \leq C_{d,\gamma} \int_{\mathbb{R}^d} V(x)_+^{\gamma+\frac{d}{2}} dx \quad \text{if } d \geq 3 \quad (3.7)$$

holds true for all $\gamma > 0$ and some constant $C_{d,\gamma}$ independent of V , see also [Fr]. This improves considerably the classical Lieb-Thirring estimates, [LT], by the presence of the negative factor $-\frac{(d-2)^2}{4|x|^2}$ on the left hand side.

Now, our Corollary 3.3 shows that the inequality

$$-\Delta_D \geq U_\infty$$

holds in the sense of quadratic forms on $H_0^1(\mathbb{R}^2 \setminus K)$. Since the constant $\frac{1}{4}$ is sharp, it is natural to ask whether an analog of (3.7) holds for the operator

$$H_D(1, U_\infty) = -\Delta_D - U_\infty$$

in $L^2(M)$ with Dirichlet boundary conditions. With the help of Theorem 2.10 we obtain

Theorem 3.4. *Let $R_{\mathrm{in}}(K) = \rho$. For every $\gamma > 0$ there exists $C(\gamma, \rho)$ such that*

$$\mathrm{Tr} (-\Delta_D - U_\infty - V)_-^\gamma \leq C(\gamma, \rho) \int_M V_+(x)^{\gamma+1} dx \quad (3.8)$$

holds true for all $V \in L^{\gamma+1}(M)$.

Proof. By the min-max principle it suffices to prove (3.8) for $V \geq 0$. The inequality of Lieb, see [L], yields the upper bound

$$\mathrm{Tr} (-\Delta_D - U_\infty - V)_-^\gamma \leq L_{b,\gamma} \int_M \int_0^\infty e^{-tH_D(1, U_\infty)}(x, x) t^{-1-\gamma} (tV(x) - b)_+ dt dx, \quad (3.9)$$

where $b > 0$ is arbitrary and

$$L_{b,\gamma} = \Gamma(\gamma + 1) \left(e^{-b} - b \int_b^\infty s^{-1} e^{-s} ds \right)^{-1}. \quad (3.10)$$

On the other hand, Theorem 2.10 implies that

$$e^{-tH_D(1, U_\infty)}(x, x) \leq C \frac{\log \frac{|x|}{\rho}}{t \log \frac{|x| + \sqrt{t}}{\rho}} \leq \frac{C}{t} \quad \forall x \in M, \quad t > 0,$$

with some constant C independent of x . Inequality (3.8) now follows by inserting the above upper bound in (3.9) and integrating with respect to t . \square

In the sequel we denote by

$$N(-\Delta_D - \lambda U_\infty - V, 0) := \mathrm{Tr} (-\Delta_D - U_\infty - aV)_-^0$$

the number of negative eigenvalues, counted with their multiplicities, of the operator $-\Delta_D - \lambda U_\infty - V$.

Remark 3.5. Inequality (3.8), similarly as (3.7), fails when $\gamma = 0$. Indeed, if for $K = B(0, \rho)$, then a standard test function argument shows that the operator $-\Delta_D - U_\infty - aV$, with some $V \geq 0$, $V \neq 0$, has at least one negative eigenvalue for any $a > 0$. Hence

$$N(-\Delta_D - U_\infty - aV, 0) \geq 1 \quad \forall a > 0,$$

which contradicts (3.8) for $\gamma = 0$ and a small enough.

If $\lambda < 1$, then the operator $H_D(\lambda, U_\infty)$ is sub-critical, and it is possible to extend inequality (3.8) to the border-line case $\gamma = 0$.

Theorem 3.6. *Assume that $R_{\text{in}}(K) = \rho = 1$. There exists a constant C_0 such that*

$$N(-\Delta_D - \lambda U_\infty - V, 0) \leq \frac{C_0}{\sqrt{1-\lambda}} \int_M V_+(x) (\log V_+(x))^{-\sqrt{1-\lambda}} (\log |x|)^{1+\sqrt{1-\lambda}} dx \quad (3.11)$$

holds true for all $0 \leq \lambda < 1$ and for all V for which the right hand side is finite.

Proof. As in the proof of Theorem 3.4 we assume without loss of generality that $V \geq 0$. Since $|x| \geq 1$, Theorem 2.10 implies that the upper bound

$$e^{-tH_D(\lambda, U_\infty)}(x, x) \leq \frac{C (\log |x|)^{1+\sqrt{1-\lambda}}}{t (\log(|x| + \sqrt{t}))^{1+\sqrt{1-\lambda}}} \leq \frac{4C (\log |x|)^{1+\sqrt{1-\lambda}}}{t (\log t)^{1+\sqrt{1-\lambda}}}$$

holds for all $x \in M$ and $t > 0$. Hence in view of (3.9) we have

$$\begin{aligned} N(-\Delta_D - \lambda U_\infty - V, 0) &\leq L_{b,0} \int_M \int_0^\infty e^{-tH_D(\lambda, U_\infty)}(x, x) t^{-1} (tV(x) - b)_+ dt dx \\ &\leq C_0 \int_M (\log |x|)^{1+\sqrt{1-\lambda}} \int_0^\infty \frac{(tV(x) - b)_+}{t^2 (\log t)^{1+\sqrt{1-\lambda}}} dt dx, \end{aligned}$$

where $C_0 = 4C L_{b,0}$. The claim follows by choosing $b = 1$ and integrating with respect to t . \square

Remark 3.7. As expected the constant on the right hand side of (3.11) diverges as λ approaches the critical value 1. The presence of a logarithmic weight in the estimates for the number of negative eigenvalues of Schrödinger operators is typical for the two-dimensional case, see e.g. [LS, So1, St].

4. The case $d = 1$

The effect of boundary conditions on the large behavior of the heat kernel in dimension one is even more robust than the case $d = 2$. In order to see why let us consider the half-line $M = \mathbb{R}_+$ and the Laplacian with Robin boundary condition at zero associated with the symmetric sesquilinear form

$$\mathcal{Q}_\sigma[u, v] = \int_0^\infty \overline{u'} v' dx + \sigma \overline{u(0)} v(0), \quad u, v \in H^1(\mathbb{R}_+), \quad \sigma > 0. \quad (4.1)$$

For definiteness we will assume that the potential U is given by

$$U(x) := \mathcal{U}_\sigma(x) := \frac{1}{4} \left(x + \frac{1}{\sigma} \right)^{-2}.$$

By mimicking the arguments of section 2.1 it is easy to verify that the form

$$\mathcal{Q}_\sigma[u, v] - \lambda \int_0^\infty U \bar{u} v dx, \quad u, v \in H^1(\mathbb{R}_+). \quad (4.2)$$

is closed for all $\lambda \in \mathbb{R}$ and that the associated operator, which we denote by $\mathcal{H}_\sigma(\lambda, U)$, generates in $L^2(\mathbb{R}_+)$ an ultracontractive semigroup with integral kernel

$$e^{-t \mathcal{H}_\sigma(\lambda, U_\sigma)}(x, y), \quad x, y \in M, \quad t > 0.$$

We have

Theorem 4.1. *Let $0 \leq \lambda \leq 1$. Then there exist positive constants $C, c > 0$ such that for all $x, y \in \mathbb{R}_+$ and all $t > 0$*

$$\frac{C F_1(x, y; \lambda) e^{-\frac{c|x-y|^2}{t}}}{\sqrt{t} \left(x + \sqrt{t} + \frac{1}{\sigma}\right)^{1+\sqrt{1-\lambda}}} \leq e^{-t \mathcal{H}_\sigma(\lambda, U_\sigma)}(x, y) \leq \frac{F_1(x, y; \lambda) e^{-\frac{|x-y|^2}{ct}}}{C \sqrt{t} \left(x + \sqrt{t} + \frac{1}{\sigma}\right)^{1+\sqrt{1-\lambda}}},$$

where

$$F_1(x, y; \lambda) = \left(\left(x + \frac{1}{\sigma}\right) \left(y + \frac{1}{\sigma}\right) \right)^{\frac{1+\sqrt{1-\lambda}}{2}}.$$

Proof. We will proceed in a similar way as in the proof of Theorem 2.6. Here we choose the weight function in the form

$$\omega(x) := \left(x + \frac{\alpha}{\sigma}\right)^\alpha, \quad (4.3)$$

with α as in (2.22), and substitute $u = \omega f$, $v = \omega g$ with $f, g \in H^1(\mathbb{R}_+, \omega^2 dx)$. A direct calculation then yields

$$\mathcal{Q}_\sigma[u, v] - \lambda \int_0^\infty \mathcal{U}_\sigma \bar{u} v dx = \int_0^\infty \bar{f}' g' \omega^2 dx.$$

Hence

$$e^{-t \mathcal{H}_\sigma(\lambda, U_\sigma)}(x, y) = \omega(x) \omega(y) e^{-t \mathcal{A}_\sigma}(x, y), \quad x, y \in \mathbb{R}_+, \quad (4.4)$$

where \mathcal{A}_σ is the self-adjoint operator in $L^2(\mathbb{R}_+, \omega^2 dx)$ associated with the quadratic form

$$\int_0^\infty |f'|^2 \omega^2 dx$$

with the form domain $H^1(\mathbb{R}_+, \omega^2 dx)$. Since

$$\sup_{0 \leq x \leq 2r} \omega(x) \leq C' \inf_{r \leq x} \omega(x), \quad \forall r > 0, \quad (4.5)$$

with C' independent of r , it follows from [GS, Thm. 2.11] that the weighted manifold $(\mathbb{R}_+, \omega^2 dx)$ satisfies the parabolic Harnack inequality. By [GS, Thm. 2.8] we thus infer that there exist positive constants C and c such that

$$\frac{C e^{-\frac{c|x-y|^2}{t}}}{\mathcal{V}_1(x, \sqrt{t})} \leq e^{-t \mathcal{A}_\sigma}(x, y) \leq \frac{e^{-\frac{|x-y|^2}{ct}}}{C \mathcal{V}_1(x, \sqrt{t})},$$

holds for all $x, y \in \mathbb{R}_+$ and $t > 0$, where

$$\mathcal{V}_1(x, \sqrt{t}) = \int_{x-\sqrt{t}}^{x+\sqrt{t}} \omega^2(y) dy.$$

Since

$$\frac{\sqrt{t}}{2^{2\alpha+1}} \left(x + \sqrt{t} + \frac{\alpha}{\sigma} \right)^{2\alpha} \leq \mathcal{V}_1(x, \sqrt{t}) \leq 2\sqrt{t} \left(x + \sqrt{t} + \frac{\alpha}{\sigma} \right)^{2\alpha},$$

the claim follows from (4.4). \square

5. The case $d \geq 3$

Contrary to the cases $d = 1$ and $d = 2$, in higher dimensions the presence of Robin boundary conditions on ∂M does not accelerate the decay of the associated heat kernel, at least as long as no potential is introduced. Indeed, using the domination of semigroups and [GS, Thm. 3.1] we obtain

Proposition 5.1. *Let $d \geq 3$ and let $K \subset \mathbb{R}^d$ be an open bounded and simply connected set with Lipschitz boundary. Let $M = \mathbb{R}^d \setminus K$. Assume that $\sigma \in L^\infty(\partial M)$. Then there exist positive constants ε , c and C such that*

$$C^{-1} t^{-\frac{d}{2}} e^{-\frac{c|x-y|^2}{t}} \leq e^{t\Delta_\sigma}(x, y) \leq C t^{-\frac{d}{2}} e^{-\frac{|x-y|^2}{ct}} \quad (5.1)$$

holds for all $t > 0$ and all $x, y \in M \setminus K_\varepsilon$.

Proof. By domination of semigroups we have

$$e^{t\Delta_D}(x, y) \leq e^{t\Delta_\sigma}(x, y) \leq e^{t\Delta_0}(x, y), \quad x, y \in M, \quad t > 0. \quad (5.2)$$

Since \mathbb{R}^d , $d \geq 3$, equipped with the Euclidean metric is a non-parabolic manifold which satisfies the parabolic Harnack inequality, we can apply [GS, Thm. 3.1]. The latter implies that

$$e^{t\Delta_D}(x, y) \geq C^{-1} t^{-\frac{d}{2}} e^{-\frac{c|x-y|^2}{t}}.$$

This proves the lower bound in (5.1). The upper bound follows from (1.2) and (5.2). \square

APPENDIX A.

Lemma A.1. *In addition to Assumption 2.1, let $K \subset \mathbb{R}^2$ have a C^2 -regular boundary. Let w be given by (2.14) with $\alpha \in [1/2, 1]$ and $\beta > 0$. Then there exists a constant c , independent of α and β , such that*

$$\sup_{x \in B(x_0, 2r)} w(x) \leq c \inf_{x \in M \setminus B(x_0, r)} w(x) \quad (A.1)$$

holds for any $x_0 \in M$ and all r large enough.

Proof. Take $\gamma > 2$ large enough so that $\overline{K} \subset B(x_0, \gamma|x_0|)$. Then for any $r \geq \gamma|x_0|$ we have

$$\sup_{x \in B(x_0, 2r)} w(x) \leq \left(\log \frac{|x_0| + 2r}{\rho} + \beta \right)^\alpha \leq \left(\log \frac{r(2 + \gamma^{-1})}{\rho} + \beta \right)^\alpha. \quad (A.2)$$

On the other hand, since $r \geq \gamma|x_0| \geq \gamma\rho$ for $c > 1$ it holds

$$\begin{aligned} c \inf_{x \in M \setminus B(x_0, r)} w(x) &\geq \left(c \log \frac{r - |x_0|}{\rho} + \beta \right)^\alpha \geq \left(c \log \frac{r(1 - \gamma^{-1})}{\rho} + \beta \right)^\alpha \\ &\geq \left(\log \frac{r}{\rho} + \log(\gamma^{c-1} (1 - \gamma^{-1})^c) + \beta \right)^\alpha, \end{aligned}$$

where we have used the fact that $1/2 \leq \alpha \leq 1$, see (2.22). In view of (A.2) it thus suffices to take c large enough such that

$$\gamma^{c-1} (1 - \gamma^{-1})^c \geq 2 + \gamma^{-1}.$$

□

Lemma A.2. *Let w be given by (2.14) with $\alpha, \beta > 0$. Then there exists a constant $c_0 > 0$, independent of β , such that*

$$c_0 t \left(\log \left(\frac{|x| + \sqrt{t}}{\rho} \right) + \beta \right)^{2\alpha} \leq \mathcal{V}_2(x, \sqrt{t}) \leq \pi t \left(\log \left(\frac{|x| + \sqrt{t}}{\rho} \right) + \beta \right)^{2\alpha} \quad (\text{A.3})$$

holds for all $x \in M$ and $t > 0$, where $\mathcal{V}_2(x, \sqrt{t})$ is defined in (2.25).

Proof. The upper bound is obvious. To establish the lower bound we first prove the following auxiliary estimate:

$$\forall \delta \in (0, 1) : \log \left(\frac{|x| + \delta s}{\rho} \right) \geq \delta \log \left(\frac{|x| + s}{\rho} \right) \quad \forall x \in M, \forall s > 0. \quad (\text{A.4})$$

Indeed, since $|x| \geq \rho$ for all $x \in M$, by the Bernoulli inequality we have

$$\left(\frac{|x| + \delta s}{\rho} \right)^{\frac{1}{\delta}} = \left(\frac{|x|}{\rho} \right)^{\frac{1}{\delta}} \left(1 + \frac{\delta s}{|x|} \right)^{\frac{1}{\delta}} \geq \frac{|x|}{\rho} \left(1 + \frac{s}{|x|} \right) = \frac{|x| + s}{\rho},$$

which implies (A.4). Next, since K is bounded there exists $k_0 > 0$ such that

$$K \subset B \left(0, \frac{k_0}{2} \right). \quad (\text{A.5})$$

Consider first the case when $|x| + \sqrt{t} > k_0$. Then there exists a circular segment $\mathfrak{B}(x, \sqrt{t})$ of $B(x, \sqrt{t})$ with height $\frac{\sqrt{t}}{2}$ and such that

$$\mathfrak{B}(x, \sqrt{t}) \subset \left(B(x, \sqrt{t}) \setminus B \left(0, |x| + \frac{\sqrt{t}}{2} \right) \right) \subset M. \quad (\text{A.6})$$

The latter implies that

$$w(y) \geq \left(\log \left(\frac{|x|}{\rho} + \frac{\sqrt{t}}{2\rho} \right) + \beta \right)^\alpha \quad \forall y \in \mathfrak{B}(x, \sqrt{t}).$$

An elementary calculation now shows that

$$\begin{aligned} \mathcal{V}_2(x, \sqrt{t}) &\geq \int_{\mathfrak{B}(x, \sqrt{t})} w^2(y) dy \geq \inf_{y \in \mathfrak{B}(x, \sqrt{t})} w^2(y) \int_{\mathfrak{B}(x, \sqrt{t})} dy \\ &= t \left(\frac{\pi}{3} - \frac{\sqrt{3}}{4} \right) \inf_{y \in \mathfrak{B}(x, \sqrt{t})} w^2(y) \\ &\geq t \left(\frac{\pi}{3} - \frac{\sqrt{3}}{4} \right) \left(\log \left(\frac{|x|}{\rho} + \frac{\sqrt{t}}{2\rho} \right) + \beta \right)^{2\alpha} \\ &\geq t \left(\frac{\pi}{3} - \frac{\sqrt{3}}{4} \right) 2^{-2\alpha} \left(\log \left(\frac{|x| + \sqrt{t}}{\rho} \right) + \beta \right)^{2\alpha}, \end{aligned} \quad (\text{A.7})$$

where we have used (A.4).

Assume now that $|x| + \sqrt{t} \leq k_0$. In this case we pick $\varepsilon > 0$ and distinguish two separate situations:

1. $x \in M \setminus B(0, \rho + \varepsilon)$. For any fixed x we consider the function

$$F_x(t) = t^{-1} \int_{B(x, \sqrt{t}) \cap M} \left(\log \frac{|y|}{\rho} \right)^{2\alpha} dy$$

as a function of t on the interval $(0, (k_0 - |x|)^2]$. This function is obviously positive and continuous. On the other hand, K satisfies exterior cone condition. By the Lebesgue property we thus have

$$\liminf_{t \rightarrow 0} F_x(t) \geq C \left(\log \frac{|x|}{\rho} \right)^{2\alpha} \geq C \left(\log \frac{\rho + \varepsilon}{\rho} \right)^{2\alpha},$$

with some constant $C > 0$ independent of x . Hence

$$\inf_{0 < t \leq (k_0 - |x|)^2} F_x(t) \geq c_\varepsilon \log \left(\frac{k_0}{\rho} \right)^{2\alpha}$$

for some $c_\varepsilon > 0$. It follows that

$$\int_{B(x, \sqrt{t}) \cap M} \left(\log \frac{|y|}{\rho} \right)^{2\alpha} dy \geq c_\varepsilon t \log \left(\frac{k_0}{\rho} \right)^{2\alpha} \geq c_\varepsilon t \log \left(\frac{|x| + \sqrt{t}}{\rho} \right)^{2\alpha} \quad (\text{A.8})$$

holds for all $x \in M \setminus B(0, \rho + \varepsilon)$ and all $t \in (0, (k_0 - |x|)^2]$.

2. $x \in M \cap B(0, \rho + \varepsilon)$. From the fact that the curvature of ∂K is bounded, by assumption, it follows that by taking $\varepsilon \leq \varepsilon_0$, with ε_0 small enough, we can ensure that there exists $\gamma \in (0, \pi)$ and a constant $\delta_\gamma \in (0, 1)$ such for any $x \in M \cap B(0, \rho + \varepsilon)$ and t small enough the ball $B(x, \sqrt{t})$ contains a circular section $B_\gamma(x, \sqrt{t}) \subset M$ with the opening angle γ which satisfies

$$\forall y \in B_\gamma(x, \sqrt{t}) : |y| \geq |x| + \delta_\gamma |x - y|.$$

We then have

$$\begin{aligned} \int_{B(x, \sqrt{t}) \cap M} \left(\log \frac{|y|}{\rho} \right)^{2\alpha} dy &\geq \int_{B_\gamma(x, \sqrt{t})} \left(\log \frac{|y|}{\rho} \right)^{2\alpha} dy \geq \frac{\gamma}{2} \int_0^{\sqrt{t}} \left(\log \frac{|x| + \delta_\gamma s}{\rho} \right)^{2\alpha} s ds \\ &\geq \frac{\gamma}{2} \int_{\sqrt{t}/2}^{\sqrt{t}} \left(\log \frac{|x| + \delta_\gamma s}{\rho} \right)^{2\alpha} s ds \\ &\geq \frac{\gamma}{2} \left(\log \frac{|x| + \frac{\delta_\gamma \sqrt{t}}{2}}{\rho} \right)^{2\alpha} \int_{\sqrt{t}/2}^{\sqrt{t}} s ds \geq C' t \log \left(\frac{|x| + \sqrt{t}}{\rho} \right)^{2\alpha}, \end{aligned}$$

where we have used (A.4). The constant $C' > 0$ here depends only on ε_0 and γ . Using the same reasoning as above we thus conclude that estimate (A.8) holds, with a different constant, also for all $x \in M \cap B(0, \rho + \varepsilon)$ and all $t \in (0, (k_0 - |x|)^2]$. Since $\frac{1}{2} \leq \alpha \leq 1$, see equation (2.22), this in combination with (A.7) shows that

$$\mathcal{V}_2(x, \sqrt{t}) \geq c_0 t \log \left(\frac{|x| + \sqrt{t}}{\rho} + \beta \right)^{2\alpha}$$

for all $x \in M$ and some c_0 . □

As a consequence of Lemma A.2 we obtain the volume doubling property of the manifold $(M, w^2 dx)$.

Lemma A.3. *Let w be given by (2.14) with $\alpha, \beta > 0$. Then*

$$\mathcal{V}_2(x, 2r) \leq \frac{4^{\alpha+1}\pi}{c_0} \mathcal{V}_2(x, r), \quad \forall x \in M, \forall r > 0,$$

where c_0 is given by Lemma A.2 and $\mathcal{V}_2(x, \sqrt{t})$ is defined in (2.25).

Proof. The claim follows by choosing $\delta = \frac{1}{2}$ in (A.4). \square

APPENDIX B.

Let w be given by (2.14) with $\alpha, \beta > 0$ and let $L^p(M, w^2 dx), p > 1$, be the space of functions f such that

$$\|f\|_{p,w}^p := \int_M |f(x)|^p w^2(x) dx < \infty.$$

We have

Lemma B.1. *For any $q \in (2, \infty)$ there exists a constant C_q such that*

$$\|f\|_{q,w} \leq C_q \|f\|_{H^1(M, w^2 dx)} \quad \forall f \in H^1(M, w^2 dx), \quad (\text{B.1})$$

where

$$\|f\|_{H^1(M, w^2 dx)} := \left(\int_M (|\nabla f|^2 + |f|^2) w^2 dx \right)^{\frac{1}{2}}.$$

Proof. Let $f \in H^1(M, w^2 dx)$ and set $u := f w^{\frac{2}{q}}$. Note that in view of (2.14)

$$\inf_{x \in M} w(x) > 0, \quad \sup_{x \in M} \frac{|\nabla w(x)|}{w(x)} < \infty. \quad (\text{B.2})$$

Since $2q > 4$ by assumption, equation (B.2) implies that for some c_0 there holds

$$\int_M |f|^2 w^{\frac{4}{q}} dx \leq c_0 \|f\|_{2,w}^2, \quad \int_M |\nabla f|^2 w^{\frac{4}{q}} dx \leq c_0 \|\nabla f\|_{2,w}^2.$$

Hence by Hölder's inequality we get

$$\begin{aligned} \int_M |\nabla u|^2 dx &= \int_M \left(|\nabla f|^2 w^{\frac{4}{q}} + \frac{4}{q} f w^{\frac{4}{q}-1} \nabla f \cdot \nabla w + \frac{4}{q^2} |f|^2 w^{\frac{4}{q}-2} |\nabla w|^2 \right) dx \\ &\leq c_0 \|\nabla f\|_{2,w}^2 + \frac{4c_0}{q} \left\| \frac{\nabla w}{w} \right\|_{L^\infty(M)} \|f\|_{2,w} \|\nabla f\|_{2,w} + \frac{4c_0}{q^2} \left\| \frac{\nabla w}{w} \right\|_{L^\infty(M)}^2 \|f\|_{2,w}^2 \\ &\leq c_1 (\|f\|_{2,w}^2 + \|\nabla f\|_{2,w}^2). \end{aligned}$$

for some c_1 . It follows that $u \in H^1(M, dx)$ and

$$\|u\|_{H^1(M, dx)}^2 \leq (c_1 + c_0) \|f\|_{H^1(M, w^2 dx)}^2. \quad (\text{B.3})$$

On the other hand, the standard Sobolev imbedding theorem, see e.g. [AdaFou, Thm. 4.12], says that there exists some K_q such that

$$\|u\|_{L^q(M, dx)} \leq K_q \|u\|_{H^1(M, dx)}.$$

Since $\|f\|_{q,w} = \|u\|_{L^q(M, dx)}$, the claim follows from (B.3). \square

Acknowledgements

H. K. was supported by the Gruppo Nazionale per Analisi Matematica, la Probabilità e le loro Applicazioni (GNAMPA) of the Istituto Nazionale di Alta Matematica (INdAM). The support of MIUR-PRIN2010-11 grant for the project “Calcolo delle variazioni” (H. K.) is also gratefully acknowledged.

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